DIMENSIONS NBS

*The magazine of the
National Bureau
of Standards
U.S. Department
of Commerce*

October 1981
FINAL ISSUE

PLAYING THE NUMBERS. See page 2.

COMMENT

TO OUR READERS

In line with reduced government spending, publication of DIMENSIONS/NBS will cease with this issue. The unused portions of subscriptions will be refunded automatically, either by check or credit. Questions on refunds should be sent to the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402.

Jan Kosko

Jan Kosko
Editor, DIMENSIONS/NBS

NBS DIMENSIONS

The magazine of the
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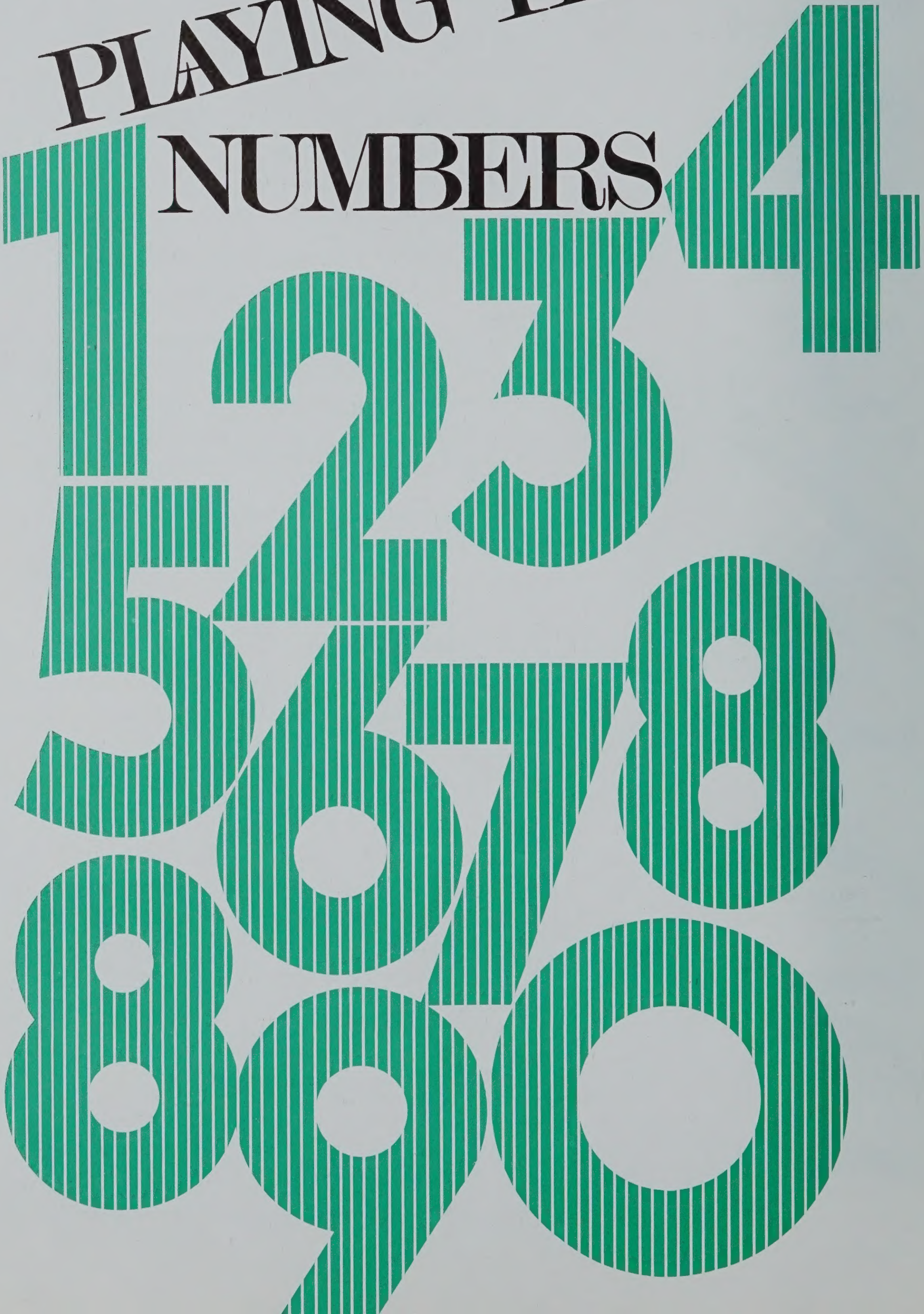
PLAYING THE NUMBERS



COVER STORY

Quantum Chemistry Finds a Place As a Broad Research Tool

by Gail Porter

MOST chemists depend on some form of hands-on experimentation to tell them what they need to know about a substance. And they have created a wide array of instruments and methods to help them: mass spectrometry, chromatography, atomic absorption and emission spectroscopy, x-ray microanalysis, calorimetry, etc-ometry.

But there is at least one brand of chemists, the quantum chemists, who rarely even see the substances they study. For the quantum chemists' instrument of choice is the computer and the tools of their trade are complex mathematical models.

Quantum chemists use mathematical models inspired by the theories of quantum mechanics to describe the energy states, sizes, shapes, and spectra of molecules or chemical systems which are either difficult or impossible to observe directly.

Some intermediate compounds, for example, says Alfons Weber, acting chief of the National Bureau of Standards Molecular Spectroscopy Division, "simply don't live long enough" to be observed with the usual spectroscopic methods (see box). In the midst of chemical reactions, individual molecular species may be created and subsequently swallowed by other compounds in less than a nanosecond (1/billionth of a second). Other species may be created at concentrations too low to be adequately detected. Yet a researcher often must know the identity and form of these species to design more efficient chemical systems or to fully understand basic chemical phenomena.

Porter is a writer and public information specialist in the NBS Public Information Division.

COUNTING ON QUANTUM CHEMISTRY

The expression is hackneyed, but that's because it's useful: "Every atom and every molecule has its own set of chemical fingerprints." That is, every atom and molecule displays its own characteristic pattern of emission or absorption of electromagnetic radiation whenever its electrons gain or lose energy.

To say it still another way, electromagnetic radiation is the legal tender of the energy business. And, like our own currency, electromagnetic radiation is measured only in specific units or quantums of value. There are $10 bills, pennies and nickels, but there is no such thing as $10.52.

Scientists can determine the identity and percentage of individual elements in a substance by measuring the intensity and frequency of the electromagnetic radiation it exchanges with its surroundings. When a piece of copper, for example, is placed in the flame of a Bunsen burner, the flame turns bright green. Individual copper atoms are gaining energy from the flame and then "relaxing" back to their preferred "ground state" by giving up the energy in the form of electromagnetic radiation. The flame turns green because most of that energy is given up in the frequency range our eyes associate with the color green.

Other elements give up most of their excess energy in the x-ray, ultraviolet, infrared, microwave or radio frequency ranges, which are not visible, but which can be detected with sensitive instruments. The pattern or full complement of radiation emitted by a compound or element is called its spectra.

Determining the spectra for molecules is much more complicated than it is for individual atoms because researchers must account for changes in vibrational as well as electronic energy levels. This is because molecules can absorb energy in two ways—by jumping electrons to higher energy orbitals or by increasing the distance between the nuclei of single atoms in the molecule. In the second case, the nuclei act like the opposite ends of a spring and the molecule resonates, giving off electromagnetic radiation at specific frequencies.

Despite the arsenal of instruments at the spectroscopist's disposal it is often quite difficult to decipher the details of a molecule's vibrational and electronic spectra, especially when dealing with complex organic or unusual compounds. This is where the quantum chemist can help. By calculating the approximate emission and absorption frequencies for a molecule, the quantum chemist can help make a spectroscopist's data more intelligible, and ultimately more useful for predicting chemical behavior.

Quantum chemistry, says Weber, allows a researcher to describe in a fundamental sense, "how molecules hang together." As such it is a flexible tool with a broad range of applications in fields such as combustion research, atmospheric chemistry and laser technology.

On the other hand, because quantum chemists rely on mathematics alone, their task of accurately calculating rather than "measuring" the characteristic energy levels in a molecule can be incredibly difficult.

"We're totally computer intensive," says Morris Krauss, leader of the NBS Quantum Chemistry Group. Without the speed of today's modern supercomputers, the field of quantum chemistry would simply not exist. Walter Stevens, another member of the NBS Quantum Chemistry Group, estimates that it costs about $5,000 in computer time to calculate the electronic and vibrational energy levels of two- or three-atom molecules. By research standards, however, such a price is quite reasonable.

In most cases, says Krauss, it would cost many times this amount to determine similar information through laboratory experiments.

Getting Down To Basics

Quantum chemistry requires massive amounts of high quality computer capacity because molecules are massively complex things to strip down and decipher. Most scientific laypersons prefer to think of molecules and atoms as microcosmic solar systems with electrons whirling around a stationary nucleus sun. In truth, this simplified picture of atomic and molecular structure bears little resemblance to current theories.

After the creation of quantum mechanics in the mid-1920's, the planetary model of atomic structure was replaced by the concept of electron clouds, and all that seemed certain became uncertain.

The modern view of the atom includes the idea that electrons are both particles and waves. Quantum mechanics, as preached by physics greats like Schrödinger, Heisenberg, Pauli, and others, provides a means of describing the wave-like behavior of atomic systems through the use of mathematics.

Just as the mathematical expression, πr^2, can be used to describe the area within a circle, the equations of quantum mechanics can be used to "visualize" the movements of electrons about a nucleus. The thing that separates quantum mechanics from the ordinary realm of geometry is the complexity of those equations.

The job of the quantum chemist is to determine the so-called "wave functions" that define the behavior of electrons in a given atom or molecule. A wave function is essentially a probability equation that states the likelihood that any one electron "orbiting" the nucleus will be found in any one place in space at any one instant. Because the electrons interact strongly through Coulombic forces, the wave function for one electron should, theoretically at least, depend on the movements of each of the other electrons in a given system.

The classic Catch 22. How can someone begin to describe something when they must know almost everything about it before uttering a word. Obviously, they can't.

The result is that quantum chemists deal with the frustration of never being able to actually solve the equations they use. "We start with one electron moving in a field of the average system," says Krauss. "Then we build toward a solution by adding into the description the simultaneous motion correlations for one electron pair at a time. We try to get a good approximation, but we never really find a true solution." What they do create are diagrams, which simulate the "boundaries" made by electrons in a given molecular system.

These diagrams and the information they yield about energy levels for both individual electrons and entire molecular systems can tell a chemist a lot about a complicated reaction or compound under study.

Take atmospheric chemistry for instance. Difficulties in projecting the rate of formation and depletion of ozone (O_3) in the upper atmosphere have plagued chemists for many years. To make such projections, researchers construct mathematical models to describe the chemistry of a given mix of atmospheric constituents under a given set of conditions. But regardless of how well these models simulate atmospheric events, the models are only as useful as the data which go into them.

In the case of ozone projections, one of the many facts researchers need to plug into their models is, how much of the sun's energy is required to break a molecule of O_2 into two single oxygen atoms. Free oxygen atoms are likely to bond rather quickly with the much more prevalent O_2 molecules to form O_3.

Several years ago, says Krauss, his group was asked to calculate the predissociation energy curves for an O_2 molecule. A dissociation curve is basically a plot of the distance between the nuclei in a molecule as a function of the energy state of that

Computers allow quantum chemists to determine more accurately the characteristic energy levels in a molecule. Here, Morris Krauss, leader of the NBS Quantum Chemistry Group, calculates the energy curve of the excited charge transfer states of xenon fluoride.

molecule. As a molecule gains energy, its nuclei push away from each other. Eventually the bond(s) between them burst and the molecule flies apart (dissociates).

In some cases a molecule will also dissociate at vibrational frequencies which normally represent bound states. Equations which describe such behavior are called predissociation curves.

Even though the O_2 molecule has been extremely well characterized over the years by spectroscopists, says Krauss, the precise details of its predissociation curves had never been fully understood. The laboratory data which had been gathered were inexplicably complex. The NBS quantum chemistry group found there was a reason for this complexity. While it had been assumed that a molecule of O_2 would have one or two predissociation curves, it was found there were in fact five different curves. Once this was known, atmospheric scientists had a more realistic picture of the molecule's expected behavior and their data made more sense.

In another project for the Air Force Office of Scientific Research, he says he was asked to help some researchers who were trying to model the chemistry that produces some of the green color associated with auroras. Krauss's calculations based on quantum mechanics disagreed by three orders of magnitude with the available experimental results. But after several more years of study and a reinterpretation of the data, the reaction rates limits are now much closer to original predictions.

A Broad Research Tool

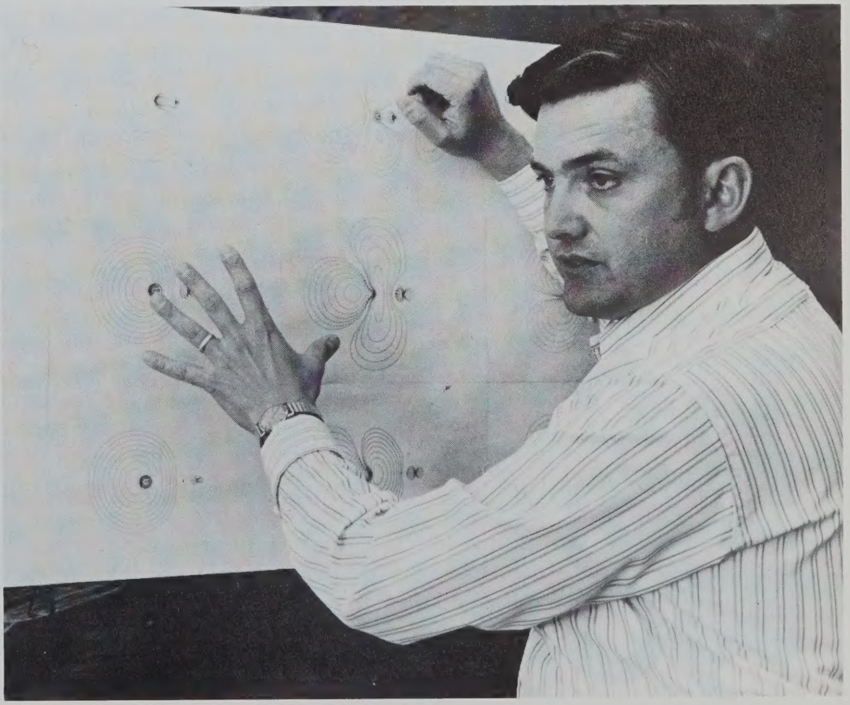
Such examples are rather rare, however. Quantum chemists make no pretense of superiority for their techniques over experimental methods. "Quantum chemists can only simulate what the spectrum looks like. Or we can help a spectroscopist to interpret data," says Krauss.

Still, in recent years, improvements in the field have been coming fast and furiously. "In 1965," says Krauss, "when I was asked to put together a compendium of all there was to know (about quantum chemistry) I could just call up my friends. I can't do that any more."

Researchers at NBS, and other national and industrial laboratories, have steadily added to the complex of algorithms, computer programs, and mathematical correction factors that make dealing with quantum calculations even feasible. There are now many major code systems, says Krauss, each of which contains hundreds of different computer programs that are applicable to quantum chemistry.

The field has developed from the plaything of a handful of physical chemists to a more broadly applicable research tool. In the past the limits on accuracy precluded dealing with heavier molecules,

Walter Stevens, a quantum chemist in the NBS Molecular Spectroscopy Division, explains various electron density maps for the lithium fluoride negative ion. Electron density maps such as these are useful for conceptualizing the results of complicated quantum chemical calculations and lead to a better understanding of the properties of the molecules being studied.



but "as time has gone on," says Krauss, "the complexity of codes has been developed to the point where such calculations can be done with some degree of ease."

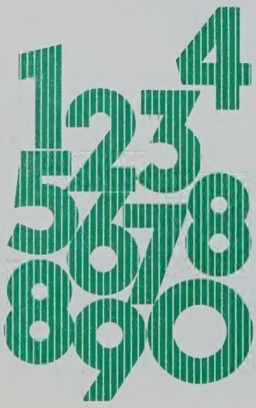
During the past several years, the NBS quantum chemistry group has been using this new capability to help the Department of Energy and the Defense Advanced Research Projects Agency (DARPA) to design laser systems for defense applications. To model adequately the transitions between energy states that occur in a laser, says Krauss, "you need a lot of very fundamental information." This is especially true for exotic molecules like xenon fluoride (XeF) or mercury bromide (HgBr) because the details of their electronic spectra are only poorly understood. Needless to say, the scientist who wants to develop laser systems based on such exotic (and expensive) molecules would do well to keep trial and error laboratory experimentation to a minimum.

In the case of xenon fluoride, the NBS Quantum Chemistry Group may have saved the DoE researchers both money and time—perhaps even years of heading in the wrong direction. The researchers knew that XeF appeared to be a good "lasing" molecule, one which could be excited and then allowed to discharge an intense pulse of ultraviolet radiation as individual molecules simultaneously "relaxed" to their ground state. But they had problems in sustaining the reaction. Although a system using XeF molecules in argon gas had worked fairly well in a prototype laser, says Krauss, the researchers were having trouble scaling up the device to provide more intense beams.

Apparently, as energy was pumped into the laser to excite the XeF molecules, the neutral argon atoms (which were being used as a buffer) would become ionized. The argon ions would then combine to form ionized argon molecules (Ar_2^+).

After calculating the respective energy curves for XeF and molecular argon ions, the NBS researchers discovered why the larger laser was not functioning properly. The frequency of emission from the XeF and the frequency for absorption for the Ar_2^+ molecules were close enough to cause interference. In the full-scale model, the longer path length of the laser put many more Ar_2^+ molecules in the path of the lasing radiation. Consequently, the argon was "eating up" the product of the lasing molecules, preventing the full radiation intensity from emerging at the end of the laser tube.

The relatively simple solution was to use a different noble gas, neon, with different absorption frequencies.



This is the beauty of quantum chemistry—the ability to understand something about the inner workings of a molecule without the complicating factors and often the expense of laboratory experimentation. Quantum chemists do not have to break down and set up new laboratories each time they begin a new project. Radically different chemical systems can be examined with the same basic tools.

The techniques of quantum chemistry, says Krauss, are particularly useful to help experimental researchers focus their work at the initial states of a project, when there is a need to answer lots of Yes/No type questions. Can a particular molecule be induced to lase or can't it? Does the emission spectrum of one molecule overlap with the absorption spectrum of another molecule in the same system, creating the possibility of interferences?

When the molecules under study are highly unstable or toxic, too refractory to be easily volatized, or otherwise difficult to work with, the use of quantum techniques becomes even more cost effective.

Until recently, the group's worst problem was not the nature of the compounds they study, or even the complexity of the computer codes they use, but the lack of access to computers with enough speed and memory to do the needed calculations.

Faced with a lack of computing capacity at NBS, Krauss used to commute routinely between NBS in Gaithersburg, Md. and NASA's Goddard Space Flight Center in Greenbelt, Md., about a 30-minute trip.

Now, however, the group has phone access to several supercomputers at Argonne National Laboratory, Lawrence Livermore Laboratory, the National Oceanic and Atmospheric Administration in Boulder, Colo., and the State University of New York at Binghamton. The computer programs or codes that translate the equations of quantum mechanics into language understood by the computer are stored on floppy disks, a kind of long-playing computer readable record. Individual sections of the disks can be read into the computer over the phone lines. This allows researchers to shift from one computer to another depending on the peak use times for different systems and on the differences in the extras like graphics programs, which are available with specific systems.

And as long as there are computers to be used there are certain to be increasingly complex problems to be solved. "During the last decade computers have become pervasive," says Krauss. "We are now able to deal with and treat quantum problems that we never even dreamed of." ☐

Meeting the Critical MATERIALS Shortage

by *John B. Wachtman, Jr.*

Technology's Role in Assuring Materials Supply

AT present, the United States imports a great many essential industrial materials. These materials provide unique and cost effective combinations of properties to many manufactured products and are currently essential in various high technology systems, including those important to national defense. Some of these, especially two of the most essential, cobalt and chromium, are concentrated overseas in areas subject to political instability. Therefore, supply disruptions of these materials are a possibility and a threat to national security. More generally, healthy economic growth depends on a continuing flow of new manufacturing processes and products based on an assured access to materials supplies. Materials technology advances can contribute to this assurance by expanding the range of supply options.

Having a national materials strategy is desirable both to deal with short term materials supply disruptions (crises) and also to encourage activities which, over the longer term, will minimize U.S. dependence on imported materials in the future.

Options For Handling A Shortage

Actions can be taken to deal with an actual or potential shortage. These can be classified as supply-oriented and technical- or performance-oriented. Supply-oriented actions include designing foreign policy to enhance the stability of foreign supplies, encouraging exploration to identify domestic sources, stockpiling, and using the Defense Production Act to establish priorities and allocations. Some performance options for dealing with a potential or actual material shortage are: first, using economical substitutions before the shortage occurs, which I shall term displacement; second, preparing for substitution with means that are presently uneconomical and actually substituting only after a shortage occurs; third, conserving through changes in design and processing; and, fourth, specialized recycling.

Displacement may occur as a result of work on substitution preparedness since a new material, now economically unattractive and suitable only as an emergency substitute, may, if prices change or technology improves, serve as a displacement before any shortage occurs. Also, developing a variety of advanced materials technologies to expand the range of approaches available to industrial designers will, over the long term, minimize import dependence.

Many new materials are being developed at present; although these advances are not primarily in response to the critical materials challenge, in many cases they do reduce dependence on imported critical materials. For example:

—Amorphous metals are coming into use because of superior magnetic properties, high strength, and high corrosion resistance.

Wachtman is director of the NBS Center for Materials Science.

— New superconducting alloys are vital to high field magnets including magnets for planned fusion energy systems.

— Surface-modified metals offer improved wear resistance, corrosion resistance, and other advantages.

— Reinforced plastics offer higher strength-to-weight and higher stiffness-to-weight ratios as well as good corrosion resistance.

— New high-temperature ceramics offer very attractive combinations of strength and oxidation resistance but pose problems of reliability.

— Advanced high-technology glasses are opening a new era of communication using optical fiber.

— Solid state electronic materials are providing vastly improved computing power.

In addition to the completely new families of materials, important new materials in the conventional field of ingot-produced alloys are coming. Two trends affecting both ingot-produced and rapidly solidified alloys are the attempts to use domestically available alloying elements, including molybdenum, nickel, vanadium, and tungsten, and to apply computer-aided alloy design.

Rapid solidification technology has opened a whole new field of alloys, both crystalline and glassy. Near-net-shape forming operations may make it possible to increase the buy-to-final use ratio, i.e., reducing the scrap produced in processing. Surface modification—new coating techniques, surface alloying, and the creation of a glassy surface layer—is a promising route to saving chromium.

The new process of very rapid quenching allows new alloy compositions to be formed. If the same composition were formed by the ingot-production process, it would separate into two or more phases with impurities in the boundaries between the phases. This can cause low corrosion resistance. Retaining all components in a single place allows desirable properties to be obtained, in some cases, with a lower content of critical materials.

An additional possibility in rapid solidification technology is to produce glassy alloys with advantageous mechanical and magnetic properties. In addition to providing hardness, the glassy structure of amorphous metals contributes to corrosion resistance. In some cases, a level of corrosion can be obtained in a particular low-chromium alloy if it is in the glassy state. An exciting possibility is to combine this result with coating technology. For example, one would like to coat steel with a low-chromium alloy rather than with pure chromium, provided the coating can be made glassy. The glassy surface layer can be made by laser pulsing or continuous wave laser scanning to melt just the near surface region.*

Another way of dealing with the critical materials problem is by producing shapes very close to the final part so only a small amount of final machining is required. Methods for doing this include powder metallurgy, precision casting, and isothermal forging. Each process, however, puts special requirements on the material in addition to the properties that they must have in service. Thus, for example, the current titanium-aluminum-vanadium alloy is not suitable for producing complex parts by hot die forging because it lacks the required ductility at the hot forging temperature. New titanium alloys have now been developed that have good forging behavior and good properties in service. Here is a case of advanced materials development that can conserve critical materials through reducing waste. This illustrates a basic theme of new materials development: a substitute material must be capable of being processed into the required parts as well as having the necessary properties.

Yet another way of meeting the critical materials challenge is specialized recycling. The high value of superalloy materials makes them good candidates for recycling, but extreme performance requirements cause stringent composition specifications. Complex alloy compositions can only be recycled into the same alloy or refined or degraded to non-superalloy use. This problem, coupled with limited refining capabilities, causes a substantial amount of superalloy scrap to be lost or degraded. Improvements in melting processes that remove carbon impurity, plus developments in refining, promise more recycling of superalloy scrap. However, the trend toward near-net-shape forming could reduce the amount of scrap and so reduce the financial incentive for installing advanced refining methods.

Although many of the critical and strategic materials are used in metallic form, there are trends toward substituting polymers or ceramics for selected applications of critical and strategic materials. The field of polymers is growing rapidly. In 1979, for the first time, the total volume of polymers used in the United States exceeded the volume of steel. Essentially all of these materials are synthetics. The emphasis in polymer development has recently

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**For more information on rapid solidification, see the article "Getting More For Less," in the July 1981 issue of DIMENSIONS/NBS.*

Metallurgist Richard Fields of the Fracture and Deformation Division inserts a creep fracture specimen into a creep machine to investigate the effects of crack on fractures at high temperatures. This procedure is being perfected and tested and will help predict the mechanical behavior of metals and ceramics under high temperatures.

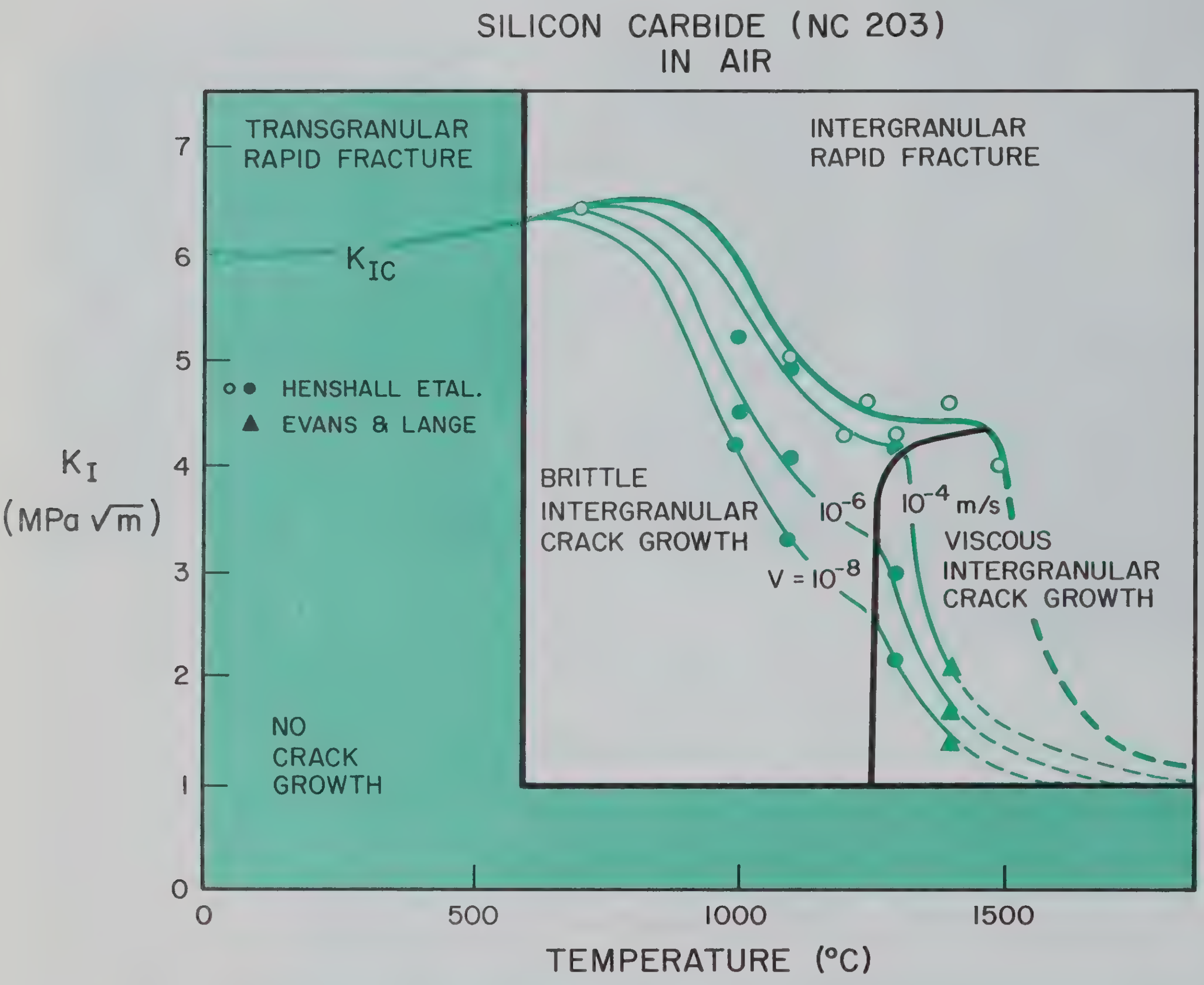
Joanne Murray, a metallurgist in the NBS Metallurgy Division, displays a typical alloy phase diagram (for the combination of iron, nickel, and chromium) on a computer terminal. NBS collects alloy phase diagrams and enters them in a computer system under a joint program with the American Society for Metals.

shifted toward producing better combinations of known polymers to give better properties and more cost effective materials. This approach allows for the maximum use of present production equipment and minimizes the requirement for new capital investment. The properties being improved include strength, high-temperature capability, controlled leaching, and electrical conductivity. High-temperature capability, needed in supersonic aircraft windows for example, is being developed in polyester carbonates so that they can replace polycarbonates which become brittle in the 80 to 120° C range.

Materials with controlled permeation and leaching are becoming very important. At one extreme, selective, high permeation is being refined for chemical separation. At the other extreme, very low permeation rates are being developed for better containment of and protection from corrosive materials. The latter could reduce critical materials requirements. So-called synthetic metals, polymers doped to produce high electrical conductivity, are a very exciting development. A new battery with polymer electrodes has been patented. New nylon block copolymers have stiffness, toughness, and impact resistance, in addition to resistance to high temperatures. Polymer blends are being perfected which combine high heat resistance and high toughness while maintaining processability. Real opportunities for replacing stainless steel with polymers exist and some are taking place, for example, in high-quality dishwasher tubs. Composites are already in widespread use where relatively low stress levels occur. These uses will be greatly increased and new high-stress uses are possible.

Exciting new developments are also taking place in the field of ceramics, many of which could help in meeting the critical materials challenge. Trends include improvements in the silicon-based family of ceramics, the toughened zirconias, glass-ceramics, oxide coatings, and electro-optic materials. The Department of Energy, the National Aeronautics and Space Administration, and General Motors are currently working together to build a ceramic turbine for automotive use. Experience gained with silicon carbide and other ceramics in this program is likely to pay off in applications to diesels and superchargers even if the turbine program does not succeed. Two-phase zirconia materials are in some ways similar to metal alloys. Their intrinsic hardness coupled with the transformation toughening produced by their two-phase structure makes them good candidates for dies. Glass ceramics can be produced very nearly in final shape by glass-forming techniques. They are then thermally treated to produce high strength and hardness and given a finish grind if necessary. They are good candidates for wear-resistant applications, especially in corrosive and high temperature conditions. Their use in gas turbines can improve performance or allow reduced use of critical materials.

This crack growth mechanism map for silicon carbide indicates regions of crack driving force (K_I) and temperature in which fracture occurs immediately, slowly, or not at all—information useful in structural design. It also identifies the micro-mechanism of fracture or crack growth which is needed to develop improved materials.



NBS Materials Program

The National Bureau of Standards program in materials reflects the Bureau's basic mission to provide infrastructure support to industry and to support the Nation's response to problems such as quality control and productivity, energy conversion, and critical materials availability.

The materials program at NBS is designed to support private industry in its search for solutions by providing measurements, standards, data, and new conceptual understanding.

The program relates to materials processing properties and durability as well as to nondestructive evaluation during processing and throughout the service life of engineering materials. Our overall program affects critical materials in two principal ways. First, it assists in the development of new, advanced materials which can displace critical materials in some applications. Second, it assists in the conservation of conventional materials by helping to reduce processing losses, improve design, and extend the lifetime of materials.

In the area of measurement technology, we are developing improved measurement methods to help industry safely, but not excessively conservatively, design structures and instruments involving alloys containing critical materials. A procedure is being perfected and tested for measuring the fracture toughness of steels and other alloys used in pipelines, pressure vessels, ships, and steels for cryogenic applications. This procedure will provide designers in large-scale construction with improved criteria for materials selection.

We measure and provide many types of data, and we operate a number of data centers which evaluate data from the literature and in some cases provide calculated estimates. The Alloy Phase Diagram Center, operated in conjunction with the American

Society for Metals, is important to the generation of substitute alloys. We are currently editing the American Society for Metal's *Phase Diagram Bulletin* and developing computer programs to aid in evaluating, plotting, and displaying phase diagrams.

NBS develops basic concepts relating processing conditions, structures, and properties. These are expressed as models to support development of improved materials or improved use of materials. For example, a fracture map has been completed for silicon carbide. In some applications, silicon carbide is a possible replacement for superalloys at high temperatures. This map, built up by piecing together individual theories and experiments, predicts different types of mechanical behavior that can be expected under various combinations of temperature and load conditions.

Previously mentioned was the potential of rapidly solidified alloys to replace critical materials in some applications. The properties of rapidly solidified alloys depend on the development of special structures and microstructures. NBS is attempting to improve conventional theory and check it by experiment to identify regions of concentration and solidification velocity favoring particular microstructures and desired properties. The improved theory should aid researchers in predicting the microstructures that will result from specific conditions and in developing industrial processes for improved materials.

Organic-matrix composites are promising materials for greater use, but problems with delamination—separation into layers—do exist, especially during impact loading. One way to reduce the possibility of delamination is through the use of rubber-modified epoxy resins. In these materials the rubber is present as tiny particles in the epoxy matrix. Measurements of fracture energy values have been made on the original resin and on the rubber-modified resin. These measurements show large increases in fracture energy for the modified resin both alone and in composites. In cooperation with the Naval Research Laboratory, we are working to improve understanding of such composites.

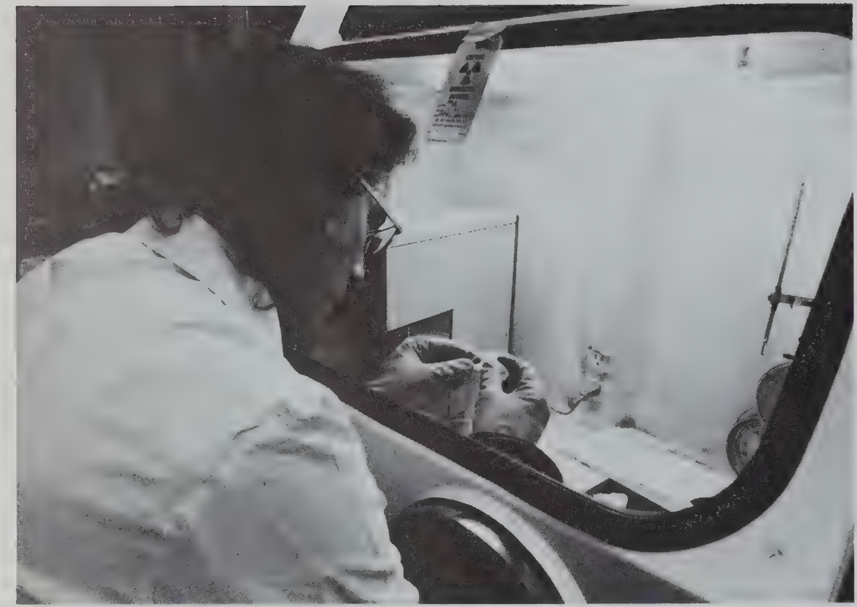
David Lashmore, the group leader of the Bureau's Electrodeposition Group, puts a specimen in an electrolyte for the pulsed electrodeposition of a nickel-chromium alloy coating. Advantages of the pulsed electrodeposition method, a surface modification process, are fine grain size, reduced hydrogen embrittlement, and more control over composition of the electrodeposited alloy.

A surface modification process (pulsed electrodeposition) under study at NBS may facilitate electrodeposition of alloy coatings of controlled composition. A common difficulty in normal electrodeposition of mixed metals is very limited control over composition of the electrodeposited alloy. In pulsed electrodeposition, an alloy can be deposited in a short pulse, avoiding this limitation. Experimental nickel-chromium alloys have been electroplated by this process; these alloys cannot be plated by the normal dc method. Additional advantages of the pulsed electrodeposition plating method are fine grain size and reduced hydrogen embrittlement. NBS is more clearly defining basic relationships among plating parameters, deposit structure, and properties.

In the case of surface modification, by using rapid solidification, an initial coating of a mixture of a metal and a hard carbide phase was formed. Results of NBS work on wear rates as a function of hardness in a variety of alloy coatings show that the wear rate goes down by more than a factor of four when coarse carbide particles are used in a cobalt-base coating rather than fine-carbide particles. This could be an opportunity for cobalt conservation.

Other current NBS activities related to critical materials include studying measurement technology and the mechanics of high temperature corrosion of alloys and alloy coatings, analyzing data on diffusion in alloys and coatings, adding to the basic science of materials durability in aggressive high temperature environments, and evaluating and publishing phase diagrams for ceramics processers and users.

In closing, I would like to emphasize that advanced materials offer many important opportunities to respond to the critical materials challenge. These responses are, however, highly specific to the particular material and application and typically involve new fundamental understanding combined with new development in processing and in design. The examples given represent some of the more promising areas; they are not intended to be exhaustive. We can look forward to new, important, and very favorable developments in advanced materials. ☐



Glass vials of the concentrated solution—one or more radionuclides dissolved in an acid—are obtained from suppliers. They are broken open, either under a fume hood or inside a glove box (as here), and the solution is removed with a small plastic squeeze bottle.

Using Natural Materials to Measure Radioactivity

by Michael Baum

HOW radioactive are you?

Not very, actually, but all parts of the human body are slightly radioactive. The world we live in is slightly radioactive, due partially to nature and partially to the work of man: it's called "background" or "environmental" radioactivity.

The level of radioactivity varies from place to place, but in general, says physicist Robin Hutchinson of the National Bureau of Standards Center for Radiation Research, a typical radioactivity concentration in soils, for example, is a few picocuries (pCi) per gram of material. (To put that somewhat in perspective, a picocurie corresponds to slightly more than 2 nuclei decaying every minute.)

Measuring radioactivity accurately at the level of a picocurie per gram or below is a difficult task, but one of interest to a wide variety of people.

Operators of nuclear power plants, for example, must meet Federal regulations in monitoring the area surrounding their facilities. They must be able to detect a 5 percent change in background radiation, which is not very large. Some plants have their own laboratories to do this work, others hire contractors.

On the other side of the regulatory fence, labs in the Environmental Protection Agency (EPA) are increasingly involved in measuring "technologically enhanced natural radiation sources," that is, materials which are naturally radioactive (such as some phosphate-bearing rocks) and have been artificially concentrated. The tailings from uranium mines are another example.

Further afield, researchers in a number of scientific disciplines use low-level radioactivity for tracing purposes or as a method of dating events. Airborne radioactive particles are collected and measured to determine how winds in the atmosphere mix and disperse pollutants; sedimentation rates in bodies of water can be deduced from the depth profile of concentrations of radioactive materials; and, of course, the radioactivity of carbon-14 is used by archaeologists to date organic remains.

Most of these people are potential customers to Hutchinson, who manages an NBS program to produce low-level radioactivity reference standards. The latest products are a new and special series of NBS Standard Reference Materials developed especially for scientists studying environmental radioactivity. "Of course, the greatest interest in these

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Baum is a public information specialist in the NBS Public Information Division.

reference materials is from people who have to meet regulatory requirements," observes Hutchinson, "but we have tried as well as we can to provide standards useful to all users."

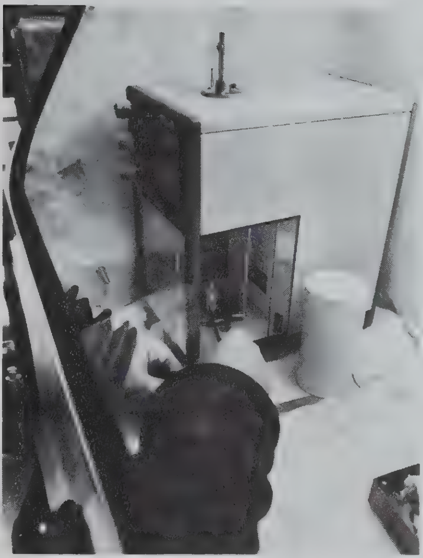
The proper and accurate measurement of radioactivity in environmental samples—such as river water or soil samples—poses problems which can tax the best laboratories, according to NBS specialists. Measurement is not just a physics problem, but one that also requires extremely selective chemical techniques.

A common approach is to take a given amount of the original sample and use chemical techniques to separate the radionuclides of interest until they are sufficiently concentrated and pure to make an accurate radioactivity measurement feasible. The activity of the original sample can then be calculated. "But there are difficult problems in analytical procedures," observes chemist Kenneth Inn at the Center for Radiation Research. "For example, in strontium separations, any calcium in the sample tends to 'follow' the radioactive strontium around quite closely, and it can interfere with the chemistry used to isolate the strontium."

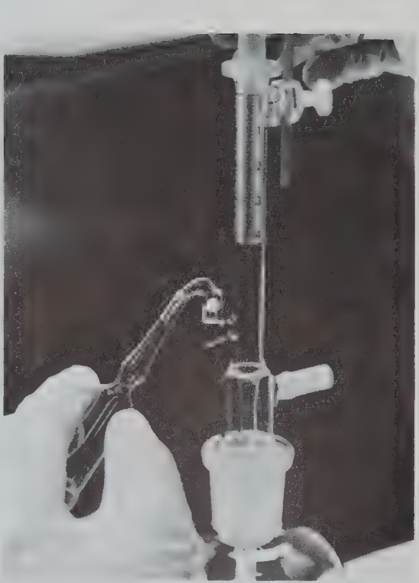
For this reason, says Inn, who specializes in low-level radioactivity analysis, a calibration which simply tests the accuracy of a radiation-detection instrument falls considerably short of assuring the accuracy of an environmental assay.

"Suppose someone is doing environmental plutonium analyses," suggests Inn, "the concentrations that would be expected are very small, so sensitive chemical separations and detection methods are needed. The sample is collected, dissolved, separated, and, once it is sufficiently pure, the plutonium is isolated in a manner which optimizes radiation detection. Testing these steps goes beyond just calibrating an instrument. You need to test the chemical procedure, the analyst's performance, and how the data are handled. You need to test the laboratory's ability to handle small amounts of radioactivity—which requires good housekeeping."

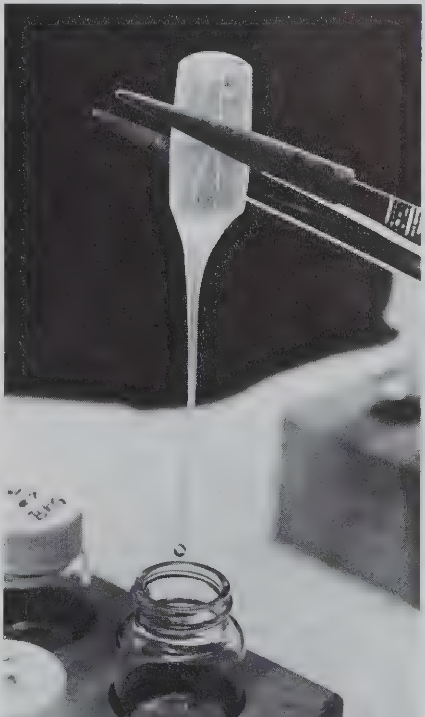
It also takes a good system to check the accuracy of the procedures, which is the purpose of the new Standard Reference Materials. An NBS Standard Reference Material (SRM) is a sample of a material which has been certified by NBS for specific chemical or physical properties. Cast steels certified for chemical composition, borax certified for hydrogen ion concentration, and point sources of plutonium-238 certified for alpha-particle radioactivity are a few examples from the catalog of more than 1000 types available.



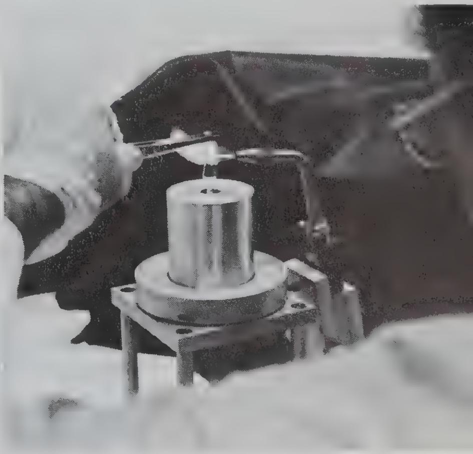
The original solution must be diluted to the strength appropriate for environmental monitoring labs. It is carefully weighed, since the dilution will be calculated from the mass of the solution.



Precisely measured amounts of the now-dilute solution are put in glass vials using this volumetric device. Lucas may prepare as many as two hundred or more vials at a time.



A certain number of test vials are also prepared to check the activity of the samples.



The glass vials are flame sealed and packaged in shock-resistant containers for shipment.

An electro-deposited thorium source, purified from a new natural matrix material, is prepared for alpha-spectrometric measurement by Kenneth Inn. Such measurements are used to determine the amount of the various alpha-emitting radionuclides in the original material.

Soil and Sediment

The new environmental radioactivity SRM's represent a relatively new type of certified reference material for radioactivity measurement applications—"natural matrix standards." They are chosen to be as close as possible to materials that an environmental analysis laboratory would be called upon to analyze from day to day. Previous radioactivity SRM's were synthesized to approximate the types of materials encountered in normal laboratory tests—carefully measured amounts of pure radioactive source material dissolved in acidic solutions or deposited on metal discs or plastic films. The "natural matrix" materials are prepared from natural sources such as soil or sediment samples, which are analyzed and certified for their radionuclide content.

These natural matrix materials are used to test the entire analysis system, says Hutchinson. They don't establish the calibration of an instrument, but the users can say that with these samples their work has been checked with NBS SRM's.

The impetus for the new line of radioactivity SRM's was the 1976 meeting of the International Committee for Radionuclide Metrology (ICRM), a worldwide organization of radiation measurement laboratories. The delegates to that meeting agreed that a series of low-level radioactivity standards in the form of naturally occurring substances was needed to provide some check of consistency of radioactivity measurements from one lab to the next. Subsequent meetings produced a list of possible "natural matrices," which were narrowed down to five substances, to be produced in the NBS Standard Reference Materials Program with the assistance of other laboratories in the ICRM.

"We will have SRM's of river sediment, lake sediment, and human tissue," says Inn. "We will have two types of soil samples, one from Peru and the other from Colorado."

The soil sample from Peru, according to Inn, was chosen because earth in the southern hemisphere typically has much less radioactivity from nuclear weapons fallout than in the northern hemisphere.

Two of the new reference materials have been completed and were recently released: river sediment from the Columbia River and soil from Rocky Flats, Colo. The other materials are in production.

Preparing the SRM's

Preparing these natural matrix SRM's raises some special challenges for the NBS laboratories. For one thing, says chemist Larry Lucas, making extremely accurate radioactivity measurements on materials with very low radioactivity is a problem. "Other typical radioactivity SRM's have an activity on the order of, say, 10 to 100 microcuries per gram," explains Lucas. "The environmental level is about a picocurie per gram, or in other words, about a million to 10-million difference. It presents a whole different world of problems."

Preparation of one of these natural matrix reference materials begins with the raw material, which typically is something as simple as a drum filled with dirt. The sample is usually provided by one of a group of interested organizations that have cooperated with NBS in the production of the new SRM's: the Nuclear Regulatory Commission, the Department of Energy's Environmental Measurements Laboratory, Woods Hole Oceanographic Institute, Oregon State University, and the Los Alamos Scientific Laboratory.

Oregon State, for example, provided the sediment from the bottom of the Columbia River that became one of the two recently issued SRM's. Samples are picked to meet a variety of criteria, one of which is that the material be easy to homogenize. (Sometimes this fails, according to Inn. Samples that are too inhomogeneous to qualify as SRM's may be released under a separate NBS program as "Research Materials," which meet somewhat less exacting criteria.)

Test vials are placed in a liquid scintillation counter, an automated test device that measures the level of radioactivity.

The materials are dried, milled to a fine powder, blended, and analyzed for whatever radionuclides are present in quantities sufficient to measure accurately. The Columbia River sediment is certified for cobalt-60, europium-152 and -154, and a number of other natural and man-made radionuclides.

A sufficient quantity of each material is prepared to last about 10 years, according to Hutchinson, which corresponds roughly to the useful lives of some of the certified radionuclides. The large supply of essentially identical samples will allow users to make long-range studies of changes in environmental radioactivity referenced to the same lot of samples. The unusually large supply of samples is another special feature of this new SRM series.

"Traceable to NBS"

The "natural matrix" SRM's are the most recent, but not the only NBS program for environmental radiation measurements. Lucas and other NBS scientists, Bert Coursey, Patricia Mullen, Francis Schima, Jackie Calhoun, and Jim Noyce (now with a private firm), have worked since 1974 on a special measurement traceability program with the EPA Environmental Monitoring and Support Laboratory (EMSL) in Las Vegas, Nev., and with the NRC Radiological and Environmental Sciences Laboratory (RESL), in Idaho Falls, Idaho.

These quality assurance laboratories run a continuing program to check the performance of a wide variety of Federal, State, local, and private laboratories that measure radioactivity in the environment. The two laboratories offer measurement systems "traceable to NBS" through two different intercomparison mechanisms, according to Lucas.

"The way the traceability programs are run," says Lucas, "is that samples are exchanged between the quality assurance laboratory and NBS, with two types of 'traceability.' In one, we send ampoules to the quality assurance laboratories. They are not told what concentration of radionuclides is in the sample, or even, in some cases, what radionuclides are in the sample. They assay the material and report back to NBS, where their results are compared with the original calibration. Different programs have different allowable deviations but typically it's about 5 percent.

"With the second method, the quality assurance laboratory sends us one of a batch of samples that it has made up—EPA and NRC furnish these sample solutions to power plants and environmental labs and so forth—and we measure that sample and issue the same sort of report. That's called 'direct traceability' of that batch of samples. We do about one traceability check a month," Lucas explains.

The radioactivity samples used in these programs are not "natural matrix" standards of the type being prepared for the SRM program, but rather are standard solutions prepared by adding carefully measured amounts of radioactive substances to some chemically stable solution. The samples are distributed either in solution (in small, sealed, glass ampoules) or dried as a small spot of radioactive material on a metal disc or between layers of plastic tape.

A wide variety of such samples has been prepared over the years to meet the needs of different types of laboratories; barium-140, mercury-203, plutonium-239, americium-241, to name a few. NBS also prepared two calibrated soil samples for the EPA program, a forerunner of the SRM project.

These traceability programs help the quality assurance laboratories to maintain the accuracy of their own laboratory intercomparisons, or "cross-check," programs. The cross-check program works roughly the same way. Participating labs receive standard radioactivity samples in one form or another from the EMSL or RESL, analyze them, and return the results to the quality assurance laboratory for comparison with all other analyses of the same sample.

The EPA also sponsors a radioactivity standards distribution program that allows any interested laboratory to obtain calibrated radioactivity standards prepared by either EMSL or NBS.

The NBS researchers hope that the new environmental radioactivity SRM's will encourage the development of more traceability programs like the EPA's program, and that this in turn will improve the quality of environmental studies. "We've begun to appreciate more the use of standards such as these in environmental studies," remarks Inn. "The use of such standards is not new, but in general it has not been widely accepted, and we want to encourage their use." ☐

SRM 4350B, River Sediment, is available in 85-gram samples, with concentrations certified for 8 radionuclides. SRM 4353, Rocky Flats Soil Number 1, is available in 90-gram samples, with concentrations certified for 13 radionuclides.

For further information, write the Office of Standard Reference Materials, B311 Chemistry Building, National Bureau of Standards, Washington, DC 20234, or phone 301/921-2045.

ON LINE WITH INDUSTRY

ALLOY PHASE DIAGRAMS: "GOING PUBLIC"

In 1978 an article in this space announced that the National Bureau of Standards was joining forces with American Society for Metals to set up a computerized data service for alloy phase diagrams. That pilot program has been successful—so much so that ASM has mounted a major fundraising drive to expand the program to a full-scale effort, one that will be self-sustaining within about 4 years through the sale of phase diagram information services. The Society estimates that the project will require some $4 million in outside funding to reach that goal.

The response to funding presentations made so far has been excellent, according to ASM funding officer J. Randy Cicen, because the metals and manufacturing industries understand the benefits of the program and are extremely interested in it. Indeed, by the close of the first week in November, the Society had firm commitments for a total of $1 million from the Cabot Corporation Foundation, Inco Limited, Battelle Memorial Institute, and the Carpenter Technology Corporation. (These companies are "Principal Associates" in the phase diagram project, signifying that they have pledged to contribute at least $50,000 annually for the next 4 years.) The fund-raising effort is directed by the ASM Resource Committee chaired by William D. Manly, senior vice-president of the Cabot Corporation.

While alloy phase diagrams are not exactly the stuff of cocktail-party conversation, they are an increasingly important form of information for industrial research and production. As the name implies, the diagrams are graphic representations of the phases or physical states that a metal or combination of metals takes at different temperatures (and sometimes pressures). The diagrams show the relationships among different metals in an alloy as temperatures and pressures change.

These are key facts in the selection of alloys for new processes or in the development of new alloys with special properties. Thus, according to metallurgists, alloy phase diagrams can save engineers a great deal of time, effort, and money—when the diagrams are available and the data are accurate.

"The lack of current, critically-evaluated phase diagrams costs the U.S. economy many millions of dollars annually," claims ASM Deputy Managing Director Edward Langer. "These costs are diffused throughout industry, and in many cases are not readily discernible. It is estimated that the data emanating from this program will save industry 5,000 times the cost of providing this data through the phase diagram program," adds Langer.

Strong words, but engineers and metallurgists in both ASM and NBS agree that good, reliable phase diagrams are essential to a variety of jobs, including finding substitutes for and recycling scarce metals, devising smelting and refining processes to make the most efficient use of metallic ore, and selecting materials for use in harsh environments or in critical applications. One speaker at the 1977 NBS workshop that helped spark the original project noted that a single copper smelter could easily waste $1 million a year in copper because of the lack of good phase diagrams for copper and copper slags.

Under the pilot program a network of up to 20 "category editors," has been funded by the NBS Metallurgy Division and the Bureau's Office of Standard Reference Data, and by others such as the Office of Naval Research, Department of Energy, and the National Science Foundation. Starting in 1978, the network began collecting data alloy phases and phase diagrams, evaluating the data for accuracy, and feeding the results to a data collection center at NBS, where the information was recorded on computer. (The NBS Metallurgy Division had established an alloy data center in 1966 and developed a system for storing the data and producing computer-drawn phase diagrams on command.)

The program now produces computer files of phase diagrams that can be drawn in different formats, depending on the need of the user, as well as publications such as the quarterly *Bulletin of Alloy Phase Diagrams,* and occasional texts published by the NBS Office of Standard Reference Data, which also helps to fund the program. Collections of phase diagrams will be published in book form by ASM. A computerized bibliographic file is in preparation.

Those interested in details of the NBS-ASM Alloy Phase Diagram Project may contact Hugh Baker, Manager, Alloy Phase Diagram Program, American Society For Metals, Metals Park, OH 44073, telephone 216/338-5151; or Robert Mehrabian, Chief, Metallurgy Division, National Bureau of Standards, Washington, DC 20234, telephone 301/921-2811. *M.B.*

STAFF REPORTS

Interface Capability, page 17
Energy Conserving, page 19
First Direct Measurement, page 21

LC/MS INTERFACE CAPABILITY EXTENDED

NBS scientists have extended the capability of the liquid chromatograph/mass spectrometer (LC/MS) interface by developing a sample introduction device to permit handling of aqueous solutions. In an early trial of the probe, analyses for valproic acid (an anticonvulsant drug) in human serum showed approximately 10 percent relative precision at the 100 ppm level.

Richard G. Christensen, Edward White V, and Harry Hertz, Organic Analytical Research Division, A113 Chemistry Building, 301/921-2154.

During the last decade, the liquid chromatograph has become an important and powerful analytical tool. Liquid chromatography can be used to separate many nonvolatile and polar molecules that are difficult or impossible to analyze by gas chromatography and can handle many compounds in matrices that are not amenable to direct gas chromatographic analysis, such as water or heavy oil. Therefore, the coupling of a mass spectrometer, a universal and/or selective detector, to a liquid chromatograph has generated a great deal of interest.

Several LC/MS interfaces have been constructed in other laboratories. Two of these methods, direct liquid injection (DLI) and evaporation onto a moving wire or belt, are now offered commercially. A system we designed and built, however, preconcentrates the liquid stream and introduces the concentrate by DLI, thereby combining advantages of both the DLI and moving belt techniques.* We have now extended the capability of the LC/MS interface by introducing a sonic probe.

The LC/MS system that we have constructed enriches the sample in the effluent of a conventional liquid chromatograph prior to its being introduced into a differentially pumped quadrupole mass spectrometer. (See Figure 1.) The effluent from the liquid chromatograph is concentrated by evaporating most of the solvent. The solvent is evaporated by allowing the effluent to flow down an electrically heated wire; the current to the wire is controlled by a feedback loop from a volume-sensing photo-cell. The concentrated effluent flows through a very small needle valve which regulates the flow into, and thereby the pressure inside, the mass spectrometer. (See Figure 2.) The valve is constructed such that the liquid is sprayed into the ion source of the mass spectrometer.

This technique has been used successfully for quantitative determinations with several chromatographic separations. For example, phenol and p-cresol were measured in samples of shale oil and solvent-refined coal. The use of the mass spectrometer as a selective liquid chromatography detector obviated the extensive sample pretreatment frequently requiring several days prior to use of other chromatographic methods of analysis, and enabled us to perform the analysis directly on the oils in about 20 minutes. We obtained relative precision of 10 percent.

Much of analytical liquid chromatography is now performed by using reversed-phase chromatography. So, to accommodate the water solutions of that mode with the LC/MS interface, we developed a new sample liquid introduction probe, which we call a sonic probe.

It is difficult to spray aqueous solutions uniformly into a vacuum because of their high surface tension and high heat of vaporization. Uniform spraying, however,

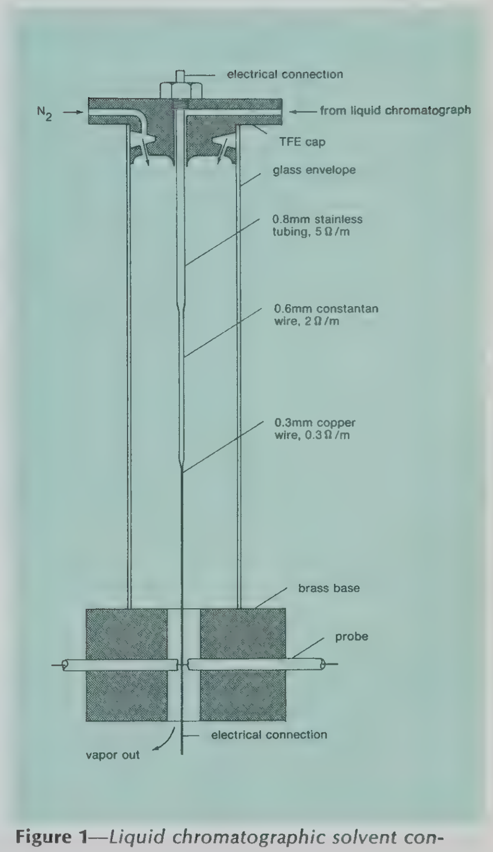

electrical connection
N_2
from liquid chromatograph
TFE cap
glass envelope
0.8mm stainless tubing, 5 Ω/m
0.6mm constantan wire, 2 Ω/m
0.3mm copper wire, 0.3 Ω/m
brass base
probe
electrical connection
vapor out

Figure 1—*Liquid chromatographic solvent concentrator wire for enrichment of the LC effluent (not drawn to scale).*

**"Liquid Chromatograph/Mass Spectrometer Interface with Continuous Sample Preconcentration," Richard G. Christensen, Harry S. Hertz, Stanley Meiselman, and Edward White V. Analytical Chemistry, Vol. 53, No. 2, February 1981.*

is necessary for quantitative results, and small droplets are required for good sensitivity with compounds of low volatility. Attempts to achieve these aims by heating the tip of the inlet tube were not successful. A sample introduction device which mechanically vibrates was constructed and has performed well (see Figure 3).

We placed a solenoid around the inlet tube which, because it is made of nickel, is magnetostrictive. An alternating field causes it to vibrate, and when it is tuned to resonance, the vibration is strong enough to cause a fog of water droplets to spray from the surface at the end of the tube. Concentrated solutions will spray without evaporative clogging, and compounds of low volatility such as adenosine can be dispersed well enough to allow molecular ion peaks to be observed.

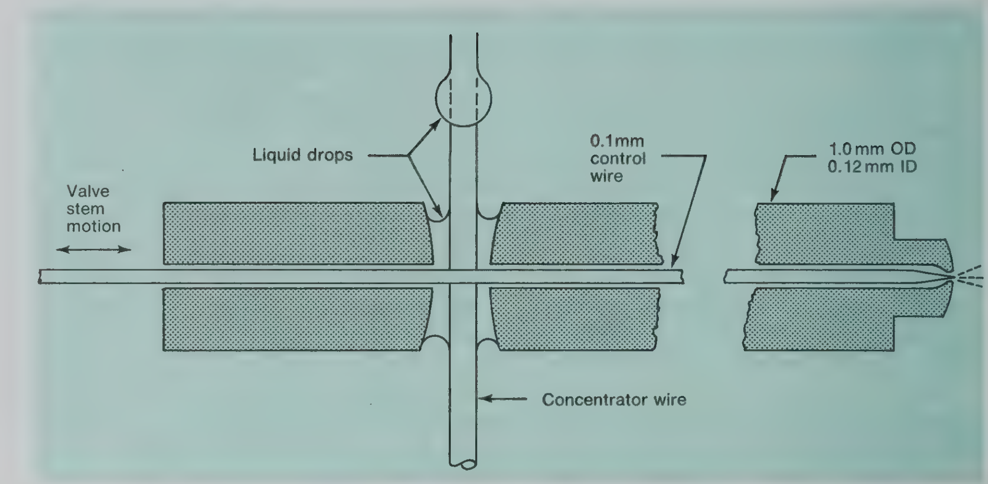


Figure 2—*Details of the direct liquid injection (DLI) probe for transfer of the concentrated eluate into a mass spectrometer.*

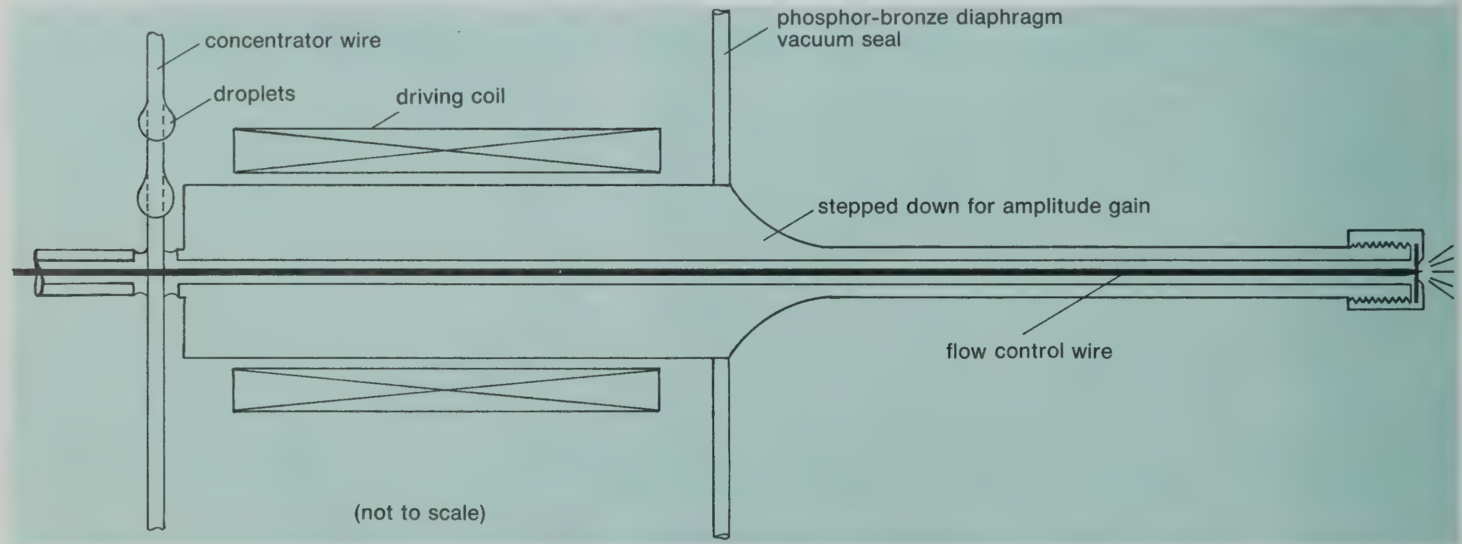

concentrator wire
droplets
driving coil
phosphor-bronze diaphragm vacuum seal
stepped down for amplitude gain
flow control wire
(not to scale)

Figure 3—*Cross-section of the "sonic probe" developed to disperse aqueous liquids into a mass spectrometer.*

NBS STUDY COMPLETED ON ENERGY CONSERVING OFFICE BUILDING

Researchers at the National Bureau of Standards Center for Building Technology recently analyzed the performance of a Manchester, N.H., Federal building and the energy conserving effectiveness of the many innovative design concepts incorporated into the building. The researchers concluded that it is possible to design an office building that uses 30-50 percent less energy than a conventional building located in the same geographic area.

James E. Hill, Building Thermal Performance Division, B114 Building Research Building, 301/921-3639.

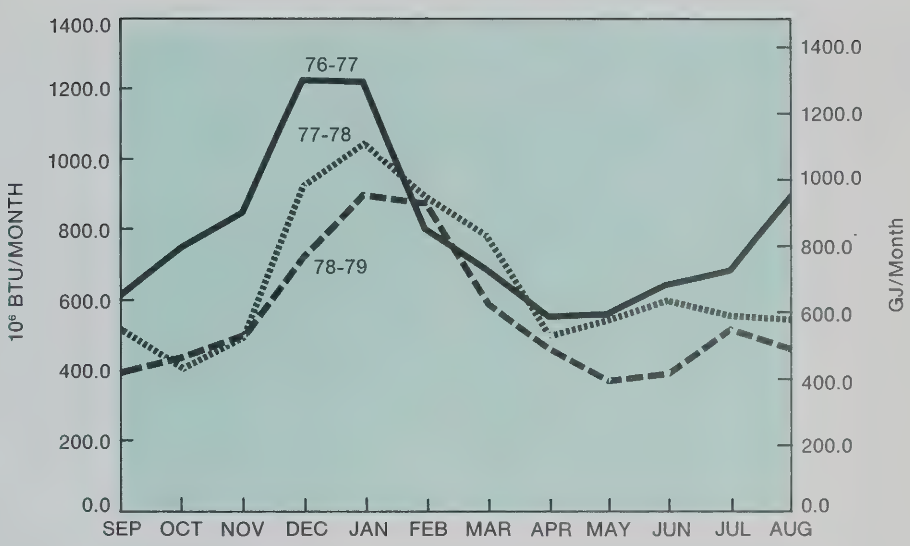


Figure 1—*Total energy consumption of the Norris Cotton Federal Office Building for the first 3 years of operation.*

The U.S. General Services Administration's Norris Cotton building was the first Federal building designed explicitly to demonstrate the potential of energy conservation design techniques. These techniques include the use of solar collectors; massive exterior walls with the insulation on the exterior side between the masonry and facial cladding to maximize the effects of thermal energy storage in the structure; small window areas to reduce heat loss (the building has no windows on the north side); and a variety of energy conserving lighting and heating, air-conditioning, and ventilation systems.

Since the building was occupied in September 1976, a team of NBS researchers, including myself; William B. May, Jr.; Thomas E. Richtmyer; Jacqueline Elder; Robert L. Tibbott; Gary T. Yonemura; Charles M. Hunt; and Phillip T. Chen from the Center for Building Technology, monitored the performance of the building. During the project we not only analyzed the building's energy consumption, but also studied the effectiveness of its many innovative design concepts. Among the areas we looked at were the building's solar system, its energy-conservation and heat recovery concepts, and its lighting systems.

In general, we found that the building performs reasonably well and proves that it is possible to design, construct, and operate a medium-sized office building in a northern climate to use no more than 625 MJ/(m^2•yr) or 55kBtu^2(ft/•yr). (See Figure 1 and Table 1.)

Since this was a new building with a unique design focusing on energy conservation, problems were experienced. However, in correcting or circumventing these problems, valuable lessons were learned and a number of conclusions were reached concerning the design and operation of an energy-conserving building.

Some of those lessons were learned regarding the design and operation of a solar system on a commercial building. The use of solar collectors demonstrated the problems of retrofitting a solar subsystem to a mechanical system that was not originally designed for it. For example, collector piping was tied into the main system in such a way that the output of the collector can go only to the basement storage tanks. If the temperature of water in the storage tanks is too low, the entire volume of water must be increased in temperature before any useful heat can be extracted. The piping design should have been modified so that the collector array energy could be used directly for meeting building loads.

We also found that under-insulated and over-sized storage tanks prevented temperatures in the tanks from reaching design levels. We recommend that thermal storage capacity in solar systems be carefully sized relative to load and solar collector capacity.

In connection with the solar collector array, we learned the importance of having compatible flat-plate solar collectors within a single system; four different flat-plate collector types are used on the Norris Cotton building. Using several types of collectors in one array both degrades the performance of the more efficient collectors and creates difficulties in flow balancing. Each type of collector has a different design flow rate. In addition, we found that changing the tilt angle of the large collector array twice a year was ineffective when the cost of the tilting mechanism and difficulty of tilting the arrays was taken into account. Changing the tilt of stationary south-facing collectors provides little advantage for space heating and domestic hot water heating applications.

We found the original solar system control scheme to be ineffective because it relied on the irradiance levels to actuate collectors without regard to ambient temperature or load.

An innovative mechanical system including solar should always have a control system whose logic can be altered by system operators. In this building, an inflexible control scheme produced undesirable sequences of equipment operation; as a result, automatic control had to be abandoned and manual control used.

As for the solar system pump speeds, the speed should not be a simple function of collector inlet and outlet temperatures. Under certain conditions such control can result in collector stagnation and boiling of the heat transfer fluid.

In addition to the findings regarding the solar system, our evaluation of the thermal energy conservation and heat recovery concept provided important lessons on the use of chilled water storage and heat recovery systems. For example, we learned that using a natural gas engine-generator to drive an electric chiller was a practical way of extracting more energy from natural gas, but using the engine waste heat to drive an absorption chiller was not.

Special care must be taken when using water-to-air coil systems with water temperatures below 41 °C (105 °F); proper design of air registers with diffusers is required to limit air velocity and avoid occupant discomfort from the relatively cool air blowing into the room.

Another problem was found with the engine-generator, electric chiller, and absorption chiller set; it did not function well as a secondary chilled water source when used in an intermittent fashion. Also, the temperature set point of the hot water heating system should have been automatically adjustable to allow for more effective use of solar-heated water.

Using chilled water storage to reduce peak cooling loads in this building was found to be ineffective due to chiller safety interlocks cycling the chiller off before design storage temperatures are reached, heat gain through tanks and long piping runs, insufficient storage capacity to meet building peak loads, and inability to automatically remove the chilled water tank from the chilled water loop when it is no longer useful.

Figure 2--Present Value Cost (1000's 1976 Dollars)

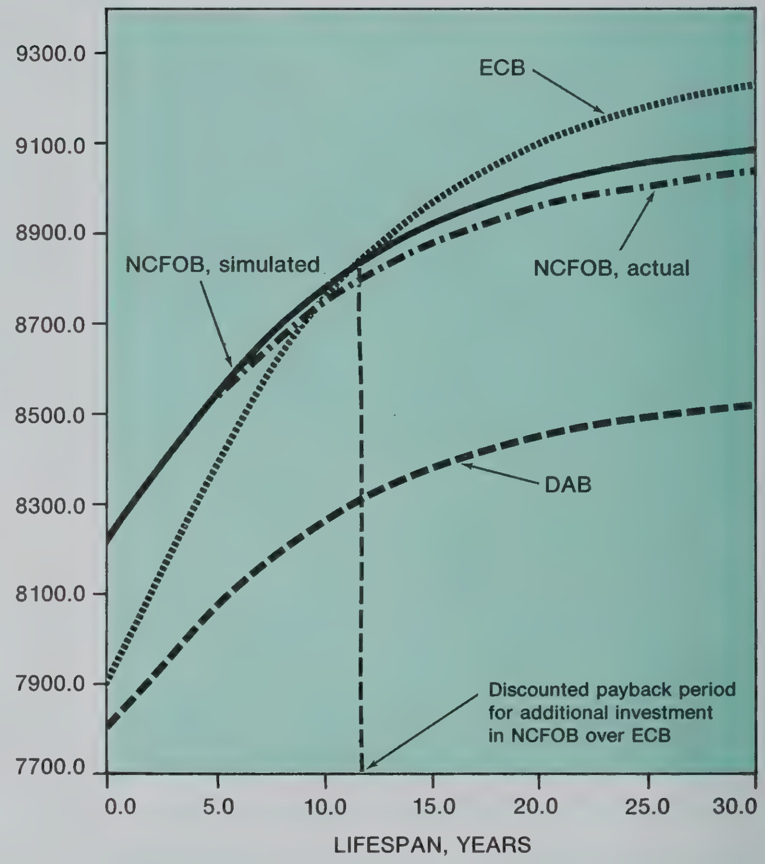


Table 1

Norris Cotton Federal Office Building Annual Energy Consumption

Year	Total energy used, MJ/m²* (Btu/ft²)*
September 76—August 77	919 (80.6 × 10³)
January 77—December 77	813 (71.3 × 10³)
September 77—August 78	758 (66.5 × 10³)
January 78—December 78	730 (64.0 × 10³)
April 78—March 79	693 (60.8 × 10³)
September 78—August 79	641 (56.2 × 10³)

*Equivalent gross floor area = 10,900 m² or (117,334 ft²).

When a heat recovery chiller (energy recovered from the condenser) is designed into a mechanical system, there must be a heating load which can be met while the chiller is required to operate, and the load must be satisfied by the fluid temperature level and flow rate from the chiller condenser. In this building, we found that heating and cooling loads occur simultaneously only for brief periods in the spring and fall. However, during these periods, the small heating loads can be met by the solar system.

Even when the ventilation system in this building was operated in a complete recirculation mode (no outside air), CO_2

levels were found to be less than the levels recommended for office space in ASHRAE Standard 62-73 (0.0118-0.0071 m^3/sec. person or 15-25 cmf/person). Also, flushing the building on summer mornings with fresh outside air to cool it below thermostat settings was found effective in reducing startup cooling load and lengthening the time before mechanical cooling was required.

A comparative study of the lighting systems used throughout the building led us to conclude that the high-pressure sodium system and one of the fluorescent systems were the most energy-effective. The task lighting system, which incorporated built-in reflective lighting on the furniture, was found to be the least effective of the experimental systems.

Six months after the building was occupied and then again 8 months later, we surveyed the building occupants to find out their likes and dislikes concerning the energy-conserving features of the building. The most positive design feature was found to be the lighting; with the exception of the occupants' strongly negative reaction to the high-pressure sodium system. Illumination level alone, however, was found not to be a good predictor of occupant response. The occupants also indicated that color rendition, glare, and amount of daylight affected satisfaction. Opinion on noise levels and disturbances was slightly more positive than negative overall. Voices were considered by the occupants to be the most disturbing noise source.

Most occupants were dissatisfied with the windows in the building because they were too small, there were too few of them, and they could not be opened.

The most negative reaction was in regard to the thermal environment. We found that ventilation levels in the building considerably exceeded ASHRAE recommendations and may have exaggerated the effects of low temperatures during the winter months. Complaints were also received concerning lower ventilation levels on the upper four floors.

Finally, based on a life-cycle cost analysis, we determined that constructing a building such as the Norris Cotton building was cost effective when it is constructed as an alternative to a Federal office building not incorporating energy conserving design features. (Although it is important to include data on operation and maintenance costs, no meaningful data on these parameters are available. Thus, our analysis includes only the building construction costs and yearly energy costs.) With certain assumptions, the discounted payback period for the building was determined to be approximately 12 years for a 30-year building lifetime. (See Figure 2.)

FIRST DIRECT MEASUREMENT OF CARBON GROUND-STATE FINE STRUCTURE

The fine-structure intervals in the ground-state multiplet of neutral carbon-12 have been measured with high accuracy by laser magnetic resonance at NBS. These precise measurements have made possible the first detection by radio astronomers of far-infrared lines from carbon-12 in several interstellar clouds.

Kenneth M. Evenson, Time and Frequency Division, 1-3530 Radio Building, National Bureau of Standards, Boulder, CO 80303, 303/497-3397.

Carbon, the fourth most abundant element in the universe, can now be studied in interstellar space in its neutral atomic form uncombined wtih other atoms. The frequencies of the fine structure intervals in the ground-state multiplets of neutral carbon-12 and carbon-13 were measured in the laboratory by using laser magnetic resonance (LMR). Radio astronomers, using the NASA Kuiper Airborne Observatory, employed these frequencies to search for far-infrared emissions from carbon contained in eight molecular clouds.

Since cold neutral carbon emits no optical radiation, its detection in interstellar space depends on far-infrared emissions. And since the frequencies of the ground-state emissions were not accurately known until we measured them, radio astronomers could not look for them.

LMR spectroscopy of neutral carbon is complicated by the difficulty of producing sufficient numbers of free atoms. We solved that problem by using a methane-fluorine atom flame inside the laser cavity. The flame products include neutral carbon, and these carbon atoms are irradiated by laser lines produced by different gases, such as CH_2F_2, DCOOD, CH_3OH, and others. The laser gain cell is pumped by a CO_2 laser. The laser lines excite the various carbon transitions when the magnetic field is scanned between 0 and 2 teslas. We can calculate the fine-structure intervals from the values of the magnetic field strength and the laser frequencies.

Our measurements give carbon-12 values of $\Delta E(^3P_2 - {}^3P_1) = 809.3446$ GHz and $\Delta E(^3P_1 - {}^3P_0) = 492.1623$ GHz with relative accuracies of 3.6×10^{-6} and 1.4×10^{-6}, respectively. Carbon-13 values need to be refined further, but the current estimates of the values are 809.346 GHz and 492.164 GHz, respectively, for the same two transitions. The measurements are about 100 times more accurate than optical measurements.

Atomic carbon in outer space may be important in cooling the gas clouds by the emission of energy in its ground state. Also, the determination of the local abundance of carbon-12 and -13 in various regions of space is of fundamental interest because the distribution of available carbon among neutral carbon (CI), singly ionized carbon (CII), and carbon monoxide (CO) has a major effect on the time-dependent and equilibrium constitution of the interstellar medium.

Radio astronomers and astrophysicists can observe these carbon emissions with ground-based instruments, instead of depending on satellites for ultraviolet observations. Further detection of these transitions in space should lead to a great deal of information about atomic abundances, isotope ratios, chemical fractionation effects, processes involving interstellar dust grains, and the general physical conditions that prevail in the interstellar medium.

INVESTIGATION OF FLORIDA CONDOMINIUM COLLAPSE COMPLETED

Lew, H. S., Carino, N. J., Fattal, S. G., and Batts, M. E., Investigation of Construction Failure of Harbour Cay Condominium in Cocoa Beach, Fla., Nat. Bur. Stand. (U.S.), NBSIR 81-2374, 107 pages (Sept. 1981). Order by Stock No. PB 82-117409 from National Technical Information Service, Springfield, VA 22161; for $12.50 prepaid.

Researchers at the National Bureau of Standards have completed their investigation into the March 27 collapse of the Harbour Cay Condominium in Cocoa Beach, Fla.

The five-story, flat-plate reinforced concrete building collapsed while under construction, killing 11 workers and injuring 23 others.

NBS conducted its investigation at the request of the U.S. Labor Department's Occupational Safety and Health Administration.

After conducting onsite technical investigations, laboratory tests, and a variety of analytical studies, NBS researchers concluded that "the most probable cause of the failure was insufficient punching shear capacity in the fifth floor slab to resist the applied construction loads."

Punching shear capacity refers to the strength of the connection between the floor slab and the supporting columns. Punching shear strength is governed by three principal factors: the strength of the concrete, the size of the columns, and the effective depth of the slab.

In the case of the Harbour Cay structure, while concrete for the roof was being placed the fifth floor slab broke away from one column, much as a blunt pencil would push through a sheet of paper.

The NBS analysis showed that "shear stresses in the slab at many column locations on the fifth floor exceeded the nominal shear strength. Thus, punching shear failure at one of the columns precipitated a progressive failure of the slab throughout the entire fifth floor. Collapse of the fifth floor, in turn, caused the successive collapse of the lower floor slabs."

Bureau researchers concluded that two factors contributed to the low punching shear capacity.

First, some of the "chairs," or supports, which hold the concrete slab reinforcing steel bars in place until the concrete has hardened, were not high enough.

Second, the design omitted a check for punching shear strength, resulting in a slab thickness of 203 mm (8 in.). A design in accordance with the American Concrete Institute 318 Standard, which is part of the local building code, would have required a thickness of 279 mm (11 in.) to provide adequate safety against punching shear under design loads. This design deficiency "resulted in a reduction of the margin of safety such that the slab had insufficient reserve strength to accommodate construction errors," the NBS report noted.

MEASURING CMOS/SOS PROCESS PERFORMANCE AND CONTROL

Linholm, L. W., The Design, Testing, and Analysis of a Comprehensive Test Pattern for Measuring CMOS/SOS Process Performance and Control, Nat. Bur. Stand. (U.S.), Spec. Publ. 400-66, 148 pages (Aug. 1981). Order by Stock No. 003-003-02345-1, from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402; for $5.50 prepaid.

With the increasing complexity of integrated circuits, it is becoming more difficult for both the manufacturer and user to characterize circuit performance fully. Functional testing alone is an impractical approach for evaluating complex circuits. As a result, greater emphasis is being placed on results from microelectronic test structures which have the potential of providing clear and unambiguous test results.

A new report from the National Bureau of Standards, *Semiconductor Technology: The Design, Testing, and Analysis of a Comprehensive Test Pattern for Measuring CMOS/SOS Process Performance and Control,* describes test-structure-based methods for process assessment, and in particular, how yield-limiting process problems can be identified and evaluated.

Test patterns NBS-16 and NBS-26 were designed for use with silicon-on-sapphire (SOS) complementary metal oxide-semiconductor (CMOS) technology. In the work reported, these patterns were implemented on wafers containing only test patterns and used to monitor a semiconductor production line. Such wafers are called process validation wafers (PVW's). They are produced along with each lot of product wafers, at the same time, using the same process steps.

Measurements from PVW's provide information useful for controlling the process line and for monitoring the quality of the output. The fact that data from the entire active area of a wafer is available provides the process engineer with important diagnostic information. The capability of generating "maps," showing the variation of a single parameter across a PVW, also permits the correlation of distributions of several different parameters and consequently may suggest unexpected links between variations in process and variations in product. These capabilities are made possible through computer control of the entire measurement and data display and reduction operation.

In addition to detailed descriptions of the test patterns, the NBS report includes test results necessary to establish baseline values of electrical parameters obtained using these test structures and recommended test procedures.

NEW MONOGRAPH ON ANTENNA THEORY AVAILABLE

Kerns, D. M., Plane-Wave Scattering-Matrix Theory of Antennas and Antenna-Antenna Interactions, Nat. Bur. Stand. (U.S.), Monogr. 162, 179 pages (June 1981). Order by Stock No. 003-003-01995-0, from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402; for $11 prepaid.

Microwave antenna engineers will be interested in a monograph just published by the National Bureau of Standards which contains significant advances in antenna theory.

Titled *Plane-Wave Scattering-Matrix Theory of Antennas and Antenna-Antenna Interactions,* the monograph provides new ways of analyzing antenna-antenna interactions. It also serves as a foundation for important new antenna measurement techniques, which have been implemented with major new testing facilities by NBS and other organizations.

The monograph was written by David M. Kerns, senior research scientist in NBS' Electromagnetic Fields Division in Boulder, Colo. Now retired, Kerns has received wide recognition for his theoretical work in support of antenna measurements. Much of his work applies to sophisticated antennas such as those used for satellite communications.

"The primary objective of this monograph is to facilitate the critical acceptance and proper application of antenna and field measurement techniques deriving more or less directly from the plane-wave scattering-matrix theory of antennas and antenna-antenna interactions. A secondary objective is to present some recent and some new theoretical results based on this theory," Kerns writes.

Ramond C. Baird, chief of the NBS antenna systems metrology program, notes that the monograph "combines an excellent introduction to microwave network analysis with a comprehensive treatment of the principles and applications of the plane-wave scattering-matrix theory of antennas."

Baird adds, "In one volume, the reader is provided with the basic information required to understand and perform a variety of accurate microwave antenna measurements—including, but not restricted to, near-field techniques—as well as the required supportive microwave circuit analyses and measurement."

BUILDING TECHNOLOGY PROJECTS SUMMARIZED

Raufaste, N., and Olmert, M., Building Technology Project Summaries 1980-1981, Nat. Bur. Stand. (U.S.), Spec. Publ. 446-5, 82 pages (July 1981). Order by Stock No. 003-003-02343-4, from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402; $4.50 prepaid.

More than 235 ongoing research projects carried out during 1980-1981 at the National Bureau of Standards Center for Building Technology are summarized in a new publication. Covering 11 prime research areas, the report lists the title and progress of the project, point of contact with CBT, and sponsor for each. The areas are:

- Building economics
- Building rehabilitation technology
- Building and community acoustics
- Lighting technology
- Building service systems performance
- Structures and foundations performance
- Earthquake hazard reduction
- Building safety
- Energy conservation in buildings
- Building thermal envelope systems and insulating materials
- Building solar systems technology.

PUBLICATIONS LISTING

Analytical Chemistry

Heinrich, K. F. J., Newbury, D. E., Myklebust, R. L., and Fiori, C. E., Eds., Energy Dispersive X-Ray Spectrometry. Proceedings of a Workshop on Energy Dispersive X-Ray Spectrometry held at the National Bureau of Standards, April 23-25, 1979, in Gaithersburg, Md., Nat. Bur. Stand. (U.S.), Spec. Publ. 604, 441 pages (June 1981) Stock No. 003-003-02333-7, $9 prepaid.

Building Technology

Raufaste, N., and Olmert, M., Eds., Building Technology Project Summaries 1980-1981, Nat. Bur. Stand. (U.S., Spec. Publ. 446-5, 82 pages (July 1981) Stock No. 003-003-02343-4, $4.50 prepaid.

Computer Science and Technology

Knoerdel, J. E., Computer Science & Technology: A Survey of Standardization Efforts of Coded Character Sets for Text Processing, Nat. Bur. Stand. (U.S.), Spec. Publ. 500-81, 50 pages (Sept. 1981) Stock No. 003-003-02355-8, $3 prepaid.

Electromagnetic Metrology

Wilson, P. F., Chang, D. C., and Ma, M. T., Excitation of a TEM Cell by a Vertical Electric Hertzian Dipole, Nat. Bur. Stand. (U.S.), Tech. Note 1037, 44 pages (Mar. 1981) Stock No. 003-003-02348-5, $2.25 prepaid.

Electronic Technology

Linholm, L. W., Semiconductor Measurement Technology: The Design, Testing, and Analysis of a Comprehensive Test Pattern for Measuring CMOS/SOS Process Performance and Control, Nat. Bur. Stand. (U.S.), Spec. Publ. 400-66, 148 pages (Aug. 1981) Stock No. 003-003-02345-1, $5.50 prepaid.

Energy Conservation and Production

Kusuda, T., and Bean, J. W., Savings in Electric Cooling Energy by the Use of a Whole-House Fan, Nat. Bur. Stand. (U.S.), Tech. Note 1138, 39 pages (May 1981) Stock No. 003-003-02317-5, $2.75 prepaid.

Streed, E., and Waksman, D., Uncertainty in Determining Thermal Performance of Liquid-Heating Flat-Plate Solar Collectors, Nat. Bur. Stand. (U.S.), Tech. Note 1140, 97 pages (Apr. 1981) Stock No. 003-003-02306-0, $4 prepaid.

Trechsel, H. R., and Launey, S. J., Criteria for the Installation of Energy Conservation Measures, Nat. Bur. Stand. (U.S.), Spec. Publ. 606, 203 pages (July 1981) Stock No. 003-003-02337-0, $6 prepaid.

Engineering, Product, and Information Standards

Bagg, T. C., Microfilm Readers, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) *84*, 4 pages (Oct. 1980).

Bagg, T. C., Optical Character Recognition (OCR) Inks, Nat. Bur. Stand. (U.S.) Fed. Info. Process. Stand. Publ. (FIPS PUB) *85*, 4 pages (Nov. 1980).

Little, J. L., Additional Controls for Use with American National Standards Code for Information Interchange, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) *86*, 4 pages, (Jan. 1981).

Shaw, J., Guidelines for ADP Contingency Planning, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) *87*, 31 pages (Mar. 1981).

Measurement Science and Technology: Physical Standards and Fundamental Constants

Shorten, F. J., Ed., NBS Reactor: Summary of Activities July 1979 to June 1980, Nat. Bur. Stand. (U.S.), Tech. Note 1142, 211 pages (May 1981) Stock No. 003-003-02314-1, $6 prepaid.

CONFERENCES

For general information on NBS conferences, contact Roger Rensberger, NBS Public Information Division, Washington, DC 20234, 301/921-2721.

ACM/NBS SYMPOSIUM

Papers are now being solicited for the 21st Annual Technical Symposium sponsored by the Association for Computing Machinery, Washington, D.C., chapter, and the National Bureau of Standards. "Computing and Government: Interactions and Achievements" is the theme of the June 17, 1982, symposium, which will be held at the NBS headquarters facility in Gaithersburg, Md.

Solicited from all branches of local, State, and Federal Government as well as industry and academia, papers may cover such topics as:

Large systems: distributed vs. centralized

Software design: how do Government and industry goals differ?

Personal computers: applications in Government?

Computer crime: legal and technical solutions?

Reliable systems: fact or fiction?

Papers reporting case histories are encouraged.

Authors should submit five double-spaced manuscripts (unpublished papers only) by January 12, 1982, to the program chairman, Eric S. Elsam, Bolt Beranek and Newman, Inc., 1300 North 17th Street, Arlington, VA 22209.

Brief (400-word) summaries on current research will also be considered. Notification of action on submissions will be sent to authors by March 5, 1982. About 20 minutes will be allowed at the symposium for presentation of full-length papers; 10 minutes for current research summaries. Proceedings will be published and papers will be refereed.

Eric W. Wolf, Bolt Beranek and Newman, Inc., is serving as general chairman of the symposium. Dennis Conti of NBS is the ACM/NBS liaison. Registration forms may be obtained from J. Stephen Schiavo, Romac & Associates, 1600 Wilson Boulevard, Suite 906, Arlington, VA 22209; phone 703/525-5160.

CONFERENCE CALENDAR

March 3
FIPS SOFTWARE DOCUMENTATION WORKSHOP, NBS, Gaithersburg, MD; sponsored by NBS; contact: Albrecht Neumann, A265 Technology Building, NBS, 301/921-3485.

March 14-18
SIXTH SYMPOSIUM ON TEMPERATURE—ITS MEASUREMENT AND CONTROL IN SCIENCE AND INDUSTRY, Washington Hilton Hotel, Washington, DC; sponsored by NBS, Instrument Society of America, and American Institute of Physics; contact: James Schooley, B130 Physics Building, NBS, 301/921-3315.

March 15-17
HUMAN FACTORS IN COMPUTER SYSTEMS, NBS, Gaithersburg, MD; sponsored by NBS and ACM; contact: Wilma Osborne, A265 Technology Building, NBS, 301/921-3485.

***March 18-19**
WORKSHOP ON STANDARDIZATION FOR SPEECH I/O TECHNOLOGY, NBS, Gaithersburg, MD; sponsored by NBS and NADC; contact: David Pallett, A123 Metrology Building, 301/921-3427.

March 22-26
FOURTH ASTM-EURATOM SYMPOSIUM, NBS, Gaithersburg, MD; sponsored by NBS and ASTM; contact: Charles Eisenhauer, C310 Radiation Physics Building, NBS, 301/921-2685.

March 29-April 2
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, NBS, Gaithersburg, MD; sponsored by NBS and Crystallographic Association; contact: Camden Hubbard, A221 Materials Building, NBS, 301/921-2921.

***April 14-16**
INTERNATIONAL WORKSHOP ON WIND TUNNEL MODELING CRITERIA AND TECHNIQUES, NBS, Gaithersburg, MD; sponsored by NBS; contact: Timothy Reinhold, B168 Building Research, 301/921-2186.

April 20-22
MECHANICAL FAILURES PREVENTION GROUP, NBS, Gaithersburg, MD; sponsored by NBS and MFPG; contact: T. Robert Shives, B120 Materials Building, NBS, 301/921-2934.

***April 26-28**
STRESS CORROSION CONFERENCE, NBS, Gaithersburg, MD; sponsored by NBS; contact: Gilbert Ugiansky, B354 Materials Building, NBS, 301/921-3132.

***May 17-19**
TRANSPORT PROTOCOL, NBS, Gaithersburg, MD; sponsored by NBS and IEEE; contact: Elizabeth Fong, B211 Technology Building, NBS, 301/921-2601.

***May 27**
TRENDS AND APPLICATIONS, NBS, Gaithersburg, MD; sponsored by NBS and IEEE; contact: Helen Wood, A209 Administration Building, NBS, 301/921-2834.

June 1-4
NEUTRON TRANSMUTATION DOPING OF SEMICONDUCTORS CONFERENCE, NBS, Gaithersburg, MD; sponsored by NBS; contact: Robert Larrabee, A360 Technology Building, NBS 301/921-3786.

June 7-9
SEVENTH INTERNATIONAL SYMPOSIUM ON ULTRASONIC IMAGING AND TISSUE CHARACTERIZATION, NBS, Gaithersburg, MD; sponsored by NBS, NIH, IEEE, and AIUM; contact: Melvin Linzer, A366 Materials Building, NBS, 301/921-2611.

***June 17**
21ST ANNUAL ACM TECHNICAL SYMPOSIUM, NBS, Gaithersburg, MD; sponsored by NBS and Association of Computing Machinery; contact: Dennis Conti, A265 Technology Building, NBS, 301/921-3485.

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NEWS BRIEFS

NBS-ADA RESEARCH DEMONSTRATES COMPOUNDS TO IMPROVE DENTAL MATERIALS. Research at NBS has found that a number of previously unused chemical compounds can help harden polymeric (plastic) materials for tooth fillings, dentures and bridges, and crowns. The compounds are tertiary aromatic amines derived from para-aminophenethanol or para-aminophenylacetic acid. For over 30 years, aromatic amines have been used as accelerators to speed the hardening of dental materials. But some of these amines either do not cause hardening rapidly enough at room temperature or yield polymers that do not stand up to the pressures of chewing and grinding and have poor coloring or discolor over time. The NBS-tested compounds improve on conventional amines in a number of ways. They can be used in lower concentrations, helping to avoid yellowing and to retain the tooth's natural shade. They promote faster hardening of the dental material and yield greater mechanical strength to resist wear. Significantly, they are believed to be nontoxic.

INTERFERENCE FOUND IN SOME SOLAR ENERGY SYSTEMS. NBS researchers recently took field measurements of electromagnetic interference from prototype homes in Las Cruces, N.M., that use photovoltaic technology to convert solar energy to household current. They found that some inverters, which convert DC to AC current, emit significant amounts of electromagnetic radiation over a broad frequency range. In some frequency bands, such as the AM broadcast band, the signal level is about 30 dB above the ambient background noise level; this is sufficient to completely eliminate the use of this band.

NBS, AIF RENEW PROGRAM FOR RADIOPHARMACEUTICAL SRM'S. To meet a widespread need for improved measurement of the characteristics of radiopharmaceuticals, NBS and the Atomic Industrial Forum (AIF) have renewed a program to produce a series of Standard Reference Materials. The program is one of several dozen under the Research Associate Program, a special mechanism for NBS-industry joint research.

SYSTEM PROVIDES RELIABLE, QUICK ACCESS TO STANDARDS PROVISIONS. Organization of Building Standards: Systematic Techniques for Scope and Arrangement (BSS 136) presents an innovative indexing and outlining method whose basic element is the classification of the provisions of a standard. The report may be ordered for $7 prepaid from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. Order by Stock No. 003-003-02363-9.

ANSI ADOPTS IGES FOR CAD/CAM DATA EXCHANGE. The Initial Graphics Exchange Specification (IGES), developed by an industry government coalition managed by NBS to facilitate the exchange of graphics and design data between disparate CAD/CAM systems has been adopted as a standard by the American National Standards Institute (ANSI). ANSI Subcommittee Y14.26 included IGES as three parts of the five-part standard Y14.26M, "Digital Representation for Communication of Product Definition Data," which was adopted on September 21. ANSI plans to advance Y14.26M for use as an international standard. A workshop on IGES will be held at NBS on December 14-16. Call 301/921-3691 for details.

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